

Formation of matter-wave soliton molecules

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We propose a method of forming matter-wave soliton molecules that is inspired by the recent experiment of Dris *et al.* [1]. In the proposed set-up we show that if two solitons are initially prepared in phase and with a sufficiently small separation and relative velocity, a bound pair will always form. This is verified by direct numerical simulation of the Gross-Pitaevskii equation and by the derivation of the exact interaction energy of two solitons, which takes the form of a Morse potential. This interaction potential depends not only on the separation but also on the relative phase of the solitons and is essential for an analytical treatment of a host of other problems, such as the soliton gas and the Toda lattice of solitons.

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Introduction. — Interactions between solitons have been the subject of intense study in the past few decades [2, 3, 4]. This was motivated both by the fundamental physics involved and by the prospects of important technological applications [5]. At the fundamental level, solitons show a dual nature by behaving as classical particles but also exhibiting their wave nature when they, for instance, scatter off each other. In particular, it was first pointed out by Karpman and Solov'ev using perturbation theory [2], by Gordon using the exact two solitons solution [3], and by Anderson and Lisak employing a variational approach [4], that at large distances the force between two solitons decays exponentially with their separation and is proportional to the cosine of their phase difference. From the applications point of view, this interaction between solitons is actually a problem since it leads, when using optical solitons in fibers as data carriers, to the destruction of the information stored in a sequences of solitons.

The exciting possibility of forming so-called soliton molecules gives yet another stimulus to the problem. Such molecules have indeed recently been realized experimentally with optical solitons by Stratmann *et al.*, who also measured the relative phase of the two solitons and studied their binding mechanism [6]. Matter-wave soliton molecules have, however, not yet been created experimentally. Theoretically, soliton molecules have been studied previously in two-dimensional Bose-Einstein condensates without [7] and with [8] dipolar interactions. In the latter case an effective molecular soliton-soliton potential was found, which results from the dipolar nature of the condensate and interlayer effects. Experimentally, bright solitons and soliton trains were observed as the remnants of a collapsing condensate that was created by using a Feshbach resonance to switch the interaction from repulsive to attractive [9]. It was found that neighboring solitons repel each other in spite of the fact that the interatomic interactions are attractive. A variational cal-

culation showed that the repulsive force is caused by a π phase difference between the solitons [10], in agreement with known result for optical solitons [2, 3, 4]. The conditions in these experiments are thus not favorable for forming bound states of solitons. Instead, if the two solitons start with a zero phase difference, they attract each other and may ultimately form a molecule. Our analysis of the soliton-soliton interaction energy shows that while this is indeed a necessary condition, it is not sufficient for soliton molecule formation. The initial separation and relative velocity need to be sufficiently small such that the interaction is not dramatically weakened by the exponential tail and the kinetic energy of the relative motion does not considerably exceed the soliton-soliton interaction energy.

An adjusted version of a recent experiment by Dris *et al.* [1] is suggested here as a possible experimental method of realizing soliton molecules in strongly elongated Bose-Einstein condensates. In the experiment of Ref. [1], a trapped bright soliton was launched onto a potential barrier at the center of a harmonic trap. Here partial transmission and reflection created two solitons, which then after half an oscillation in the trap recombine again into a single one. We will show, however, that a soliton molecule can be formed if both the harmonic trapping potential and the potential barrier are switched off at the time when the two solitons reach their classical turning points. This guarantees the relative velocity to be zero. Moreover, the two solitons are also guaranteed to have a zero relative phase then, since they were created coherently from the same soliton. The separation between the solitons prepared in this way is controlled by the curvature of the harmonic trap. Thus, it appears that all the conditions for soliton molecule formation can be met in such an experimental set-up. In the following, we show that this is indeed the case via direct numerical simulations of the Gross-Pitaevskii equation. This is then followed by an analytical analysis of the soliton-

soliton interaction energy, which also confirms the feasibility of our proposal. Moreover, finding an accurate interaction potential for two solitons at an arbitrary separation, is important not only for the present problem of forming soliton molecules, but may also lay the grounds for a host of other problems involving solitons interactions such as the soliton Toda lattice [11] and the soliton gas [12].

Soliton molecule formation. — The evolution of solitons in the original experiment of Ref. [1], as well as in our modified proposal, can be described by the effectively one-dimensional Gross-Pitaevskii equation (GPE)

$$\left[i \frac{\partial}{\partial t} + \frac{1}{2} \frac{\partial^2}{\partial z^2} - V_{\text{ext}}(z) + g |\Psi(z, t)|^2 \right] \Psi(z, t) = 0, \quad (1)$$

where, here and throughout, lengths are scaled to the characteristic length $a_z = \sqrt{\hbar/m\omega_z}$ of the harmonic potential $m\omega_z^2 z^2/2$, time to $1/\omega_z$, and the wavefunction $\Psi(z, t)$ to $1/\sqrt{2a_z\omega_\perp/\omega_z}$, with ω_z and ω_\perp the axial and radial frequencies of the strongly elongated ($\omega_\perp \gg \omega_z$) trapping potential, respectively. In these units, the strength of the interatomic interaction will be given by the ratio $g = -a/a_z$, where a is the s -wave scattering length. A square or gaussian potential barrier is added to the harmonic potential at the center that is included in $V_{\text{ext}}(z)$.

We now show that Eq. (1) indeed accounts for the interesting recombination of the two returning solitons at the center, as can be seen in Fig. 1(a). Repeating this simulation for the case that we switch off the harmonic trapping potential and the potential barrier at the point when the two solitons reach their classical turning points, results in the formation of a molecule of two solitons, as shown clearly in Fig. 1(b). The relative intensities or densities of the two solitons in the molecule are set by the initial velocity of the single original soliton and the height of the potential barrier.

In another version of this experiment, one can also think of phase imprinting one of the two solitons once it reaches the classical turning point. In such an experiment, the phase of the cycle performed by the molecule is controlled. For instance, one can imprint a π phase difference leading initially to an increase of the separation of the solitons. If their initial separation is small enough, however, they will ultimately return back and form the molecule since their relative phase will change from π to zero as they move away from each other and the force becomes attractive, as will be shown next.

Soliton-soliton interaction energy. — As mentioned in the introduction, the interaction energy of two solitons depends on their separation and on their relative phase. It is also known that such an interaction may lead to the formation of a bound state of two solitons. The key point here is that dynamically the relative phase of two solitons changes as their separation changes. If two solitons, that are initially in phase, approach each other sufficiently

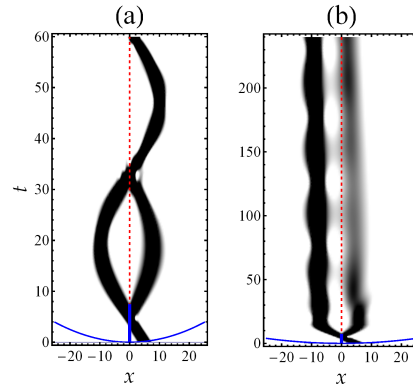


FIG. 1: (Color online) Spacio-temporal density plots for (a) the experiment of Ref. [1] and (b) our proposal for soliton molecule formation. In (a) a single soliton is split by the potential barrier into two solitons that upon returning to the trap center recombine into the original one. In (b) the harmonic trapping potential and the potential barrier, shown with the solid blue curve, are switched off at $t = 15.75$ when the two solitons reach the classical turning point. Initial soliton parameters: velocity = -0.8 , amplitude = 0.8 , position = 5 , and interaction strength $g = 0.0113$. Square barrier's parameters: height = 0.75 and width = 0.5 .

slowly, their relative phase changes such that the force between them becomes repulsive. When the two solitons then move away from each other, the force becomes attractive again and the cycle completes itself. Thus, the manner by which the relative phase changes with the separation between the solitons is essential for understanding their binding properties. This fact is qualitatively understood in the literature, but has never before quantitatively been captured in a formula that accurately gives the interaction potential of the solitons for both short as well as large separations. Here, we arrive at this objective by deriving the exact dependence of the phase, and hence the interaction potential, on the solitons separation. In addition to being of importance by itself, this potential provides a convenient analytical understanding for the possibility of soliton molecule formation.

Using the Inverse Scattering Method, the exact two soliton solution of the homogeneous version of Eq. (1) is derived in Ref. [3]. In Ref. [13], a re-derivation puts the solution in terms of 8 parameters, namely the two initial center-of-mass positions $z_{1,2}$ of the solitons, their center-of-mass velocities $v_{1,2}$, their phases $\Phi_{1,2}$, and their square amplitudes $n_{1,2}$. The separation between the solitons can then be extracted analytically, from which also the force follows in terms of these parameters. Here, we extend this formalism to derive the interaction energy and to show that it takes the form of a Morse potential.

For simplicity, the relative velocity is set to zero and the limit of nearly equal soliton densities $n_- = n_2 - n_1 \ll$

$n_+ = n_2 + n_1$ is taken. The separation $\Delta(t)$ between the solitons and their relative phase $\Phi(t)$ turn out to be given by

$$\Delta(t) = \frac{4}{\alpha} \log \left[\frac{\alpha (\alpha^2 + 2\alpha\beta \cos(\omega t + \Phi_0) + \beta^2)}{\beta g^2 n_-^2} \right], \quad (2)$$

and

$$\begin{aligned} \Phi(t) = & \tan^{-1} \left(\frac{\beta \sin(\omega t + \phi_0)}{\alpha + \beta \cos(\omega t + \phi_0)} \right) \\ & - \tan^{-1} \left(\frac{\alpha \sin(\omega t + \phi_0)}{\beta + \alpha \cos(\omega t + \phi_0)} \right), \end{aligned} \quad (3)$$

where $\beta = \exp(\alpha x_0/4)$, $\omega = \alpha g n_-/8$, and $\alpha = g n_+$. In addition, x_0 and ϕ_0 are two constants that can be determined from the initial conditions $\Delta(0) = \Delta_0$ and $\Phi(0) = \Phi_0$. The equations of motion for Δ and Φ can now be obtained by differentiating twice with respect to t . The resulting equations are simplified by inverting Eqs. (2) and (3) to express $\cos(\omega t + \phi_0)$ and $\sin(\omega t + \phi_0)$ in terms of Δ and Φ . Finally, we obtain in this manner

$$\ddot{\Delta} = -\frac{\alpha^3}{8} e^{-\frac{1}{4}\alpha\Delta} \cos \Phi, \quad (4)$$

$$\ddot{\Phi} = \frac{\alpha^4}{32} e^{-\frac{1}{4}\alpha\Delta} \sin \Phi, \quad (5)$$

which are identical to Gordon's formulae [3]. Here, however, we have the exact solutions of these equations of motion, namely Eqs. (2) and (3). This allows for obtaining the force $\ddot{\Delta}$ in terms of Δ by solving Eq. (2) for $\cos(\omega t + \phi_0)$ and substituting the solution in Eq. (4). Integrating the resulting expression with respect to Δ leads to the soliton-soliton potential energy $V_{ss} = -\int \ddot{\Delta} d\Delta$

$$V_{ss} = \frac{(\alpha^2/4) \cos \Phi_0}{e^{\frac{1}{4}\alpha\Delta_0} - e^{\frac{1}{4}\alpha\Delta_{eq}}} \left(e^{-\frac{1}{2}\alpha(\Delta - \Delta_{eq})} - 2e^{-\frac{1}{4}\alpha(\Delta - \Delta_{eq})} \right), \quad (6)$$

which has the form of a Morse potential with an equilibrium position at Δ_{eq} given by

$$\Delta_{eq} = \Delta_0 + \frac{4}{\alpha} \log \left(\frac{\alpha^2 - 2\alpha\beta \cos \Phi_0 + \beta^2}{\alpha^2 + \beta^2} \right). \quad (7)$$

Here, $\beta = \beta(\Delta_0, \Phi_0)$ corresponds to the real solution of the initial conditions.

Alternatively, the potential can be determined from the exact solution directly. To that end, the location of the two solitons are calculated numerically from the density $|\Psi(z, t)|^2$, from which the solitons separation and the associated acceleration are computed. Integrating the resulting force numerically, we again obtain an interaction potential. In Fig. 2, we plot the interaction potential obtained by the two methods. It is clear from this figure that the numerics captures the main features of the

potential in Eq. (6) apart from a slight change in the location of the equilibrium point and depth of the potential. The change is due to the fact that the difference in the center-of-mass positions is numerically difficult to define uniquely and is therefore not exactly equal to the parameter Δ in the exact solution when the two solitons are too close together and interference effects take place. The shape of this potential, specifically the existence of a global minimum, proves that a bound state of two solitons can be formed provided the initial separation and relative phase are such that the energy is negative.

Finally, we notice that both the equilibrium point and depth of the potential depend on the initial conditions. For further clarification of this rather unusual situation, we plot in Fig. 3 the solitons separation $\Delta(t)$ and relative phase $\Phi(t)$ during one period of the molecule's oscillation. It is clear that by increasing the initial separation, the equilibrium point around which the solitons oscillates also increases. Notice that, for both cases, the phase changes from 0 to π over half the period π/ω of the molecule's oscillation, which means that the force changes from attractive to repulsive over the same period of time. On the other hand, the dynamics of $\Delta(t)$ depends on Δ_0 since for larger Δ_0 there is initially a smaller overlap between the solitons and thus they will approach each other more slowly. By the time the force has changed sign, the solitons of the molecule with larger Δ_0 have a final separation that is larger than the one with smaller Δ_0 , but both have now to start moving away from each other, which amounts to different equilibrium points. We have also checked that the same conclusions are drawn directly from the exact solution of the GPE.

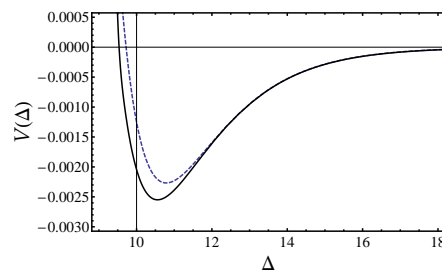


FIG. 2: Interaction potential between two bright solitons in terms of their separation. Solid curve is obtained numerically from the exact two solitons solution of the Gross-Pitaevskii equation. Dashed curve corresponds to formula (6). Parameters: $n_- = 0.2$, $n_+ = 4.7$, $g = 0.5$, $\Phi_0 = 0$.

Other applications. — Having an analytic formula for the interaction potential as a Morse potential, it is appealing to considering further applications. In particular, we can consider a classical gas of solitons interacting with the Morse potential in Eq. (6). Here, the thermodynamics is expected to be enriched by the dependence of the potential on the relative phase of the solitons.

The equation of state of such an imperfect gas

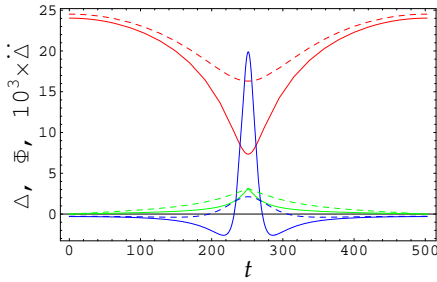


FIG. 3: (Color online) Two upper red curves: solitons separation $\Delta(t)$. Two middle green curves: phase difference $\Phi(t)$. Two lower blue curves: force $\dot{\Delta}(t)$. Time range corresponds to one period of the molecule's oscillation. Two values of the initial separation were used: $\Delta_0 = 24.0$ (solid curves) and $\Delta_0 = 24.5$ (dashed curves). Parameters: $\Phi_0 = 0$, $n_- = 0.1, n_+ = 1, g = 1$.

can be derived by a virial expansion $P/k_B T = \rho + B_2 \rho^2 + B_3 \rho^3 + \dots$, where ρ is the number density and B_2 and B_3 are the second and third virial coefficients. The second virial coefficient is given in terms of the two-body partition function which reduces to the following integration on the soliton-soliton potential: $-(1/2) \int [\exp(-V_{ss}/k_B T) - 1] d\Delta$. Due to the fact that V_{ss} depends on the initial conditions and in the partition function all configurations should be taken into account, an additional integral on all possible initial conditions should be performed. A simpler but equivalent approach is using the potential that corresponds to Eq. (4), namely $V_{ss} = -(\alpha^2/2) \exp(-\alpha \Delta/4) \cos \Phi$, where Φ is treated as an independent thermodynamic variable and the initial conditions are absent from the potential. In the limit of weak interactions $\alpha \ll k_B T$, a simple expression can be derived $B_2 = -(\pi/8)\alpha^3/(k_B T)^2$, which leads to the equation of state

$$\frac{P}{k_B T} = \rho - \frac{\pi}{8} \frac{\alpha^3}{(k_B T)^2} \rho^2. \quad (8)$$

Exploring the possibility of a phase transition to a *soliton liquid* requires extending the virial expansion to the third virial coefficient, which involves three-body processes and hence requires the knowledge of the three solitons solution, which is beyond the scope of this Letter.

As another interesting application, we briefly consider a Toda lattice of solitons, which was successfully used to model the dynamics of a train of N -solitons in external potentials [14]. The force on the i -th soliton at position z_i will be given by

$$\ddot{z}_i = F_{ss}(\Delta_{i+1}) - F_{ss}(\Delta_{i-1}), \quad (9)$$

where $\Delta_{i+1} = z_{i+1} - z_i$, $\Delta_{i-1} = z_i - z_{i-1}$, and $F_{ss} = -dV_{ss}/d\Delta$. The ground state of such a system will be a series of equidistant solitons with peak intensities alternating between two slightly different values. The value of

n_- cannot be arbitrarily small since the nearest-neighbor separation between the solitons in the lattice diverges as $\log n_-$ [13]. On the other hand, n_- should be small enough that the solitons are sufficiently separated and that the coalescence condition $n_+ g = 1$ is avoided [13]. In this configuration the net force on any soliton will vanish and the lattice moves as a rigid object that can be considered as a “soliton of solitons”. Collective excitations and sound waves can be considered as the low-energy excitations.

In conclusion, we have shown that a molecule of two bright solitons can be realized in attractive Bose-Einstein condensates. This was demonstrated both by numerical simulations and by showing that the interaction potential between the two solitons is of a molecular type and takes the form of a Morse potential. Applications of this potential in the problems of soliton gas and Toda lattice of solitons were pointed out.

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